Very Low Temperature X-ray Diffraction Study of Large Cage Zeolite Type Structures	X3A1

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Recently a number of new zeolite type structures with very large cages interconnected by multidimensional 12 ring channels were reported (1). Much interest concerns the specific structure directing mechanism that governs the assembly of such materials. Understanding of the assembly mechanism requires precise knowledge of the position of the structure directing ammines inside the large cavities of the final product. In the previous study the position of the structure directing linear ammine could not be resolved, and we therefore decided to conduct a very low temperature study in order to quench possible dynamic disorder.

We have measured extensive X-ray diffraction data at 28 K on MnxAl1-xPO4, which adopts the UCSB-8 framework structure containing a huge 64 T-atom cage. Below a summary of experimental and crystallographic details is given. The structural refinements reveal that the metal atom (Mn2+ and Al3+) distribution is highly selective. Such a metal atom site selectivity is related to the orientation of the structure directing ammines, i.e. the positively charged head groups (NH4+) of organic ammines are directed towards the most negative region of the inorganic framework (MnO2 2-) sites. There is, however, not sufficient evidence for the ordering of the hydrophobic portion of the ammine molecules. This seems to suggest that the polyether diamines may have similar structure directing effects as regular ammines.

(1) X. Bu et al, Science (1997), 278, 2080.

Experimental details: Spacegroup = P4/nnc, a = 19.200 , b = 26.628 , Temperature = 28 K, No. measured reflections = 46831, No. unique reflections = 5994, R1(36255 refs/4298 means) = 0.042, R2 = 0.054.